

Schrödinger operator on the zigzag half-nanotube in magnetic field.

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February 24, 2010

Abstract

We consider the zigzag half-nanotubes (tight-binding approximation) in a uniform magnetic field which is described by the magnetic Schrödinger operator with a periodic potential plus a finitely supported perturbation. We describe all eigenvalues and resonances of this operator, and their dependence on the magnetic field. The proof is reduced to the analysis of the periodic Jacobi operators on the half-line with finitely supported perturbations.

1 Introduction

After their discovery [Li], carbon nanotubes remain in both theoretical and applied research (see [SDD]). Structure of nanotubes are formed by rolling up a graphene sheet into a cylinder. Such nanomodels were introduced by Pauling [Pa] in 1936 to simulate aromatic molecules. They were described in more detail by Ruedenberg and Scherr [RS1] in 1953. Various physical properties of carbon nanotubes can be found in [SDD].

Single-wall nanotubes, one atomic layer in thickness in the radial direction, are a very important variety of carbon nanotube because they exhibit important electric properties that are not shared by the multi-walled carbon nanotube variants. Single-wall nanotubes are the most likely candidate for miniaturizing electronics beyond the micro electromechanical scale that is currently the basis of modern electronics.

We consider the Schrödinger operator $H^b = H_0^b + V + Q$ on the zigzag half-nanotube $\Gamma \subset \mathbb{R}^3$ (1D tight-binding model of zigzag single-wall half-nanotubes, see [SDD], [N]) in a uniform magnetic field $\mathcal{B} = |\mathcal{B}|\mathbf{e}_0$, $\mathbf{e}_0 = (0, 0, 1) \in \mathbb{R}^3$. Here H_0^b is the Hamiltonian of the nanotube in the magnetic field, V is the periodic potential of the nanotube, Q is the finitely supported perturbation.

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There are numerous mathematical results about Schrödinger operators on carbon nanotubes (zigzag, armchair and chiral) (see for example [KL], [KL1], [K1], [KuP], [Pk]). All these papers consider the so called continuous models. But in the physical literature the most commonly used model is the tight-binding model. In the tight binding model for a solid-state lattice of atoms, it is assumed that the full Hamiltonian H of the system may be approximated by the Hamiltonian of an isolated atom centered at each lattice point. The mathematical models, e.g., the Schrödinger operator on the zigzag and armchair nanotubes and ribbons in a uniform magnetic field \mathcal{B} and in an external periodic electric potential were considered in [KK1], [KK1], [Pk], see also [RR]. For applications of our models see references in [ARZ], [Ha], [SDD].

Our model nanotube Γ is a graph (see Fig. 1 and 2) embedded in \mathbb{R}^3 oriented in the z -direction \mathbf{e}_0 with unit edge length. Γ is a set of vertices (atoms) \mathbf{r}_ω connecting by bonds (edges) $\Gamma_{n,j,k}$ and

$$\begin{aligned} \Gamma &= \cup_{\omega \in \mathcal{Z}} \mathbf{r}_\omega, \quad \mathbf{r}_{n,0,k} = \mathbf{r}_{n+2k} + \frac{3n}{2}\mathbf{e}_0, \quad \mathbf{r}_{n,1,k} = \mathbf{r}_{n,0,k} + \mathbf{e}_0, \\ \omega &= (n, j, k) \in \mathcal{Z} = \mathbb{Z}_+ \times \{0, 1\} \times \mathbb{Z}_N, \quad \mathbb{Z}_N = \mathbb{Z}/(N\mathbb{Z}), \quad \mathbf{r}_k = R(\cos \frac{\pi k}{N}, \sin \frac{\pi k}{N}, 0), \\ R &= \frac{\sqrt{3}}{4 \sin \frac{\pi}{2N}}, \quad \mathbb{Z}_+ = \{j \in \mathbb{Z}, j \geq 0\}. \end{aligned} \quad (1.1)$$

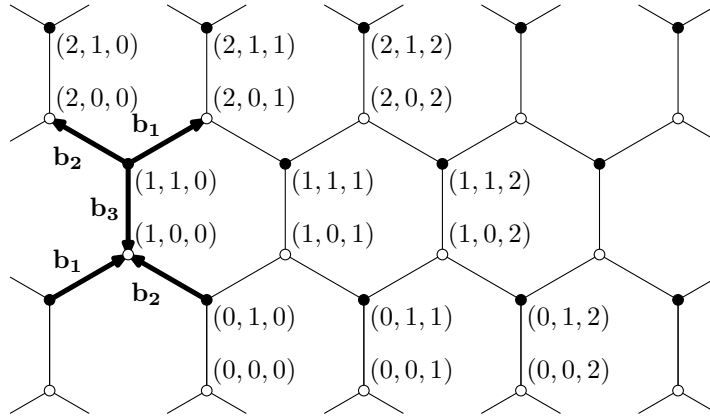


Fig 1. A piece of a nanotube.

Our carbon model nanotube is the honeycomb lattice of a graphene sheet rolled into a cylinder. This nanotube Γ has N hexagons around the cylinder embedded in \mathbb{R}^3 . Here $n \in \mathbb{Z}$ labels the position in the axial direction of the tube, $j = 0, 1$ is a label for the two types of vertices (atoms) (see Fig. 1), and $k \in \mathbb{Z}_N$ labels the position around the cylinder. The points $\mathbf{r}_{0,1,k}$, $k \in \mathbb{Z}_N$ are vertices of the regular N -gon \mathcal{P}_0 and $\mathbf{r}_{1,0,k}$ are the vertices of the regular N -gon \mathcal{P}_1 . \mathcal{P}_1 arises from \mathcal{P}_0 by combination of the rotation around the axis of the cylinder \mathcal{C} by the angle $\frac{\pi}{N}$ and of the translation by $\frac{1}{2}\mathbf{e}_0$. Repeating this procedure we obtain Γ .

Introduce the Hilbert space $\ell^2(\Gamma)$ of functions $f = (f_\omega)_{\omega \in \mathcal{Z}}$ on Γ equipped with the norm $\|f\|_{\ell^2(\Gamma)}^2 = \sum_{\omega \in \mathcal{Z}} |f_\omega|^2$. The tight-binding Hamiltonian H^b on the half-nanotube Γ has the form $H^b = H_0^b + \tilde{V}$ on $\ell^2(\Gamma)$, where H_0^b is given by (see [KL1])

$$\begin{aligned} (H_0^b f)_{n,0,k} &= e^{ib_1} f_{n-1,1,k} + e^{ib_2} f_{n-1,1,k+1} + e^{ib_3} f_{n,1,k}, & f_{-1,1,k} &= 0, \\ (H_0^b f)_{n,1,k} &= e^{ib_1} f_{n+1,0,k-1} + e^{ib_2} f_{n+1,0,k} + e^{-ib_3} f_{n,0,k}, & f &= (f_\omega)_{\omega \in \mathcal{Z}}, \\ \omega &= (n, j, k) \in \mathbb{Z}_+ \times \{0, 1\} \times \mathbb{Z}_N, & b_3 &= 0, \quad b_1 = -b_2 = b = \frac{3|\mathcal{B}|}{16} \cot \frac{\pi}{2N}, \end{aligned} \quad (1.2)$$

and the operator $\tilde{V} = V + Q$ is given by

$$(\tilde{V}f)_\omega = \tilde{V}_\omega f_\omega, \quad \text{where} \quad \tilde{V}_{n-1,1,k} = \tilde{v}_{2n}, \quad \tilde{V}_{n,0,k} = \tilde{v}_{2n+1}, \quad \tilde{v} = (\tilde{v}_n)_{n \in \mathbb{N}} \in \ell^\infty, \quad (1.3)$$

where $\tilde{v}_n = v_n + q_n$ for $0 \leq n \leq p$, $q_p \neq 0$, and $\tilde{v}_n = v_n$ for $n > p$.

Such models can be realized using optical methods, by gating, or by an acoustic field (see [N]). For example, if an external potential is given by $A_0 \cos(\xi_0 z + \beta_0)$ for some constant A_0, ξ_0, β_0 , then we obtain

$$v_{2n} = A \cos \left(2\pi \xi \left(n - \frac{1}{3} \right) + \beta \right), \quad v_{2n+1} = A \cos(2\pi \xi n + \beta), \quad n \in \mathbb{N} = 1, 2, \dots,$$

for some constant A, ξ, β . If ξ is rational, then the sequence v_n , is periodic for $n \in \mathbb{N}$. If ξ is irrational, then the sequence v_n $n \in \mathbb{Z}_+$ is almost periodic.

We give the physical sense of the finitely supported potential $q = (q_n)_{n=0}^\infty$, $q_p \neq 0$ and $q_n = 0$ for all $n > p$. There are two physical cases: a local defect in the nanotube and an effective potential. The effective potential is related to the boundary after cutting an infinite nanotube into two pieces. The effective potential is due to an imperfection in the structure of the half-nanotube near the cut and corresponds to perturbations q with p small. This motivates our detailed analysis of the properties of eigenvalues and resonances in the special case $p = 1$, $p = 2$, in Section 5.

In the present paper we suppose that the periodic background potential v has period 2 and is given by $v_{2n+1} = -v_{2n} = v \in \mathbb{R}$, $n \in \mathbb{N}$.

We formulate the result proven in [KK2] in the form convenient for us
Each operator H^b , $b \in \mathbb{R}$, is unitarily equivalent to the operator $\oplus_1^N J_k^b$, where J_k^b is the Jacobi operator, acting on $\ell^2(\mathbb{N})$ and given by

$$(J_k^b y)_n = a_{n-1} y_{n-1} + a_n y_{n+1} + \tilde{v}_n y_n, \quad (\text{for } n \geq 2), \quad (J_k^b y)_1 = a_1 y_2 + \tilde{v}_1 y_1 \quad (1.4)$$

$$a_{2n} \equiv a_{k,2n} = 2|c_k(b)|, \quad a_{2n+1} \equiv a_{k,2n+1} = 1, \quad c_k(b) = \cos(b + \frac{\pi k}{N}), \quad n \in \mathbb{N},$$

$$\tilde{v}_n = v_n + q_n, \quad q_j = 0 \text{ for } j > p, \quad q_p \neq 0, \quad (1.5)$$

and $J_k^{b+\frac{\pi}{N}} = J_{k+1}^b$, $J_k^{-b} = J_{N-k}^b$ for all $(k, b) \in \mathbb{Z}_N \times \mathbb{R}$. Moreover, the operators $H^{\pm b}$ and $H^{b+\frac{\pi}{N}}$ are unitarily equivalent for all $b \in \mathbb{R}$.

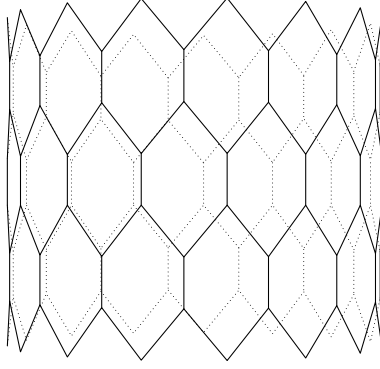


Fig 2. Nanotube in the magnetic field.

Remarks. 1) Note that the $n = 1$ case in 1.4 can be thought of as forcing the Dirichlet condition $y(0) = 0$. Thus, eigenfunctions must be non-vanishing at $n = 1$ and eigenvalues must be simple.

2) The matrix of the operator J_k^b is given by

$$J_k^b = \begin{pmatrix} \tilde{v}_1 & 1 & 0 & 0 & \dots \\ 1 & \tilde{v}_2 & 2|c_k| & 0 & \dots \\ 0 & 2|c_k| & \tilde{v}_3 & 1 & \dots \\ 0 & 0 & 1 & \tilde{v}_4 & \dots \\ 0 & 0 & 0 & 2|c_k| & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}. \quad (1.6)$$

If $c_k = \cos(b + \frac{\pi k}{N}) = 0$, then matrix (1.6) has the form

$$J_k^b|_{c_k=0} = \mathcal{J} = \begin{pmatrix} \tilde{v}_1 & 1 & 0 & 0 & \dots \\ 1 & \tilde{v}_2 & 0 & 0 & \dots \\ 0 & 0 & \tilde{v}_3 & 1 & \dots \\ 0 & 0 & 1 & \tilde{v}_4 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} = \oplus_{n \in \mathbb{N}} \mathcal{J}_n, \quad \mathcal{J}_n = \begin{pmatrix} \tilde{v}_{2n-1} & 1 \\ 1 & \tilde{v}_{2n} \end{pmatrix}, \quad (1.7)$$

with the eigenvalues

$$\{z_{n,\pm} = v_n^+ \pm |v_n^{-2} + 1|^{\frac{1}{2}}, \quad v_n^{\pm} = \frac{\tilde{v}_{2n-1} \pm \tilde{v}_{2n}}{2}, \quad n \in \mathbb{N}\}. \quad (1.8)$$

Moreover, if $q_p \neq 0$, then

if p is even, then there are at most p eigenvalues $z_{n,\pm}$, $n = 1, 2, \dots, \frac{p}{2}$,

if p is odd, then there are at most $p + 1$ eigenvalues $z_{n,\pm}$, $n = 1, 2, \dots, \frac{(p-1)}{2}$.

Note that for some special choice of perturbations $\{q_1, \dots, q_p\}$ we can have $z_i^{\pm} = z_j^{\pm}$ for $i \neq j$.

As perturbations have finite support, then there are always two flat bands (two eigenvalues with infinite multiplicities) given by $z_{n,\pm} = \pm |v^2 + 1|^{\frac{1}{2}}$, where $n \geq \frac{p}{2} + 1$ if p is even or $n \geq \frac{(p+1)}{2} + 1$ if p is odd. The flat bands are inherited from the pure periodic problem.

3) If $|c_k| = \frac{1}{2}$, then J_k^b is the Schrödinger operator with $a_n = 1$ for all $n \in \mathbb{N}$. In particular, if $b = 0$, $\frac{N}{3} \in \mathbb{N}$, then $J_{\frac{N}{3}}^0$ is the Schrödinger operator.

4) Exner [Ex] obtained some duality between Schrödinger operators on graphs and certain Jacobi matrices, which depend on energy. In our case the Jacobi matrices do not depend on energy.

Unperturbed operator. We start with the unperturbed operator $H_0^b + V$, which is unitary equivalent to $\oplus_1^N J_k^{b,0}$. The operator $J_k^{b,0}$ is acting in $\ell^2(\mathbb{N})$ with Dirichlet boundary condition, see (1.4), where $\tilde{v}_n = v_n$ is the two-periodic potential verifying $v_{2n+1} = -v_{2n} = v \in \mathbb{R}$. It is known that, if $c_k \neq 0$, then the absolutely continuous spectrum of $J_k^{b,0}$ is given by two bands and the bound states in γ_k^+ (see Section 2):

$$\begin{aligned} \sigma_{ac}(J_k^{b,0}) &= [z_{k,0}^{b,+}, z_{k,0}^{b,-}] \setminus \gamma_{k,1}^b, & \gamma_{k,1}^b &= (z_{k,1}^{b,-}, z_{k,1}^{b,+}), \\ z_{k,0}^{b,\mp} &= \pm \sqrt{v^2 + (2|c_k| + 1)^2}, & z_{k,1}^{b,\pm} &= \pm \sqrt{v^2 + (2|c_k| - 1)^2}, \quad k \in \mathbb{Z}_N, \\ \sigma(J_k^{b,0}) &= \sigma_{ac}(J_k^{b,0}) \cup \sigma_{pp}(J_k^{b,0}), & \sigma_{pp}(J_k^{b,0}) &= \begin{cases} \{v\} & \text{if } 1/2 < |c_k| \leq 1, \\ \emptyset & \text{if } 0 < |c_k| \leq 1/2, \end{cases} \end{aligned} \quad (1.9)$$

where $\gamma_{k,1}^b$ is the middle gap in the spectrum of $J_k^{b,0}$. We denote $\gamma_0 = (-\infty, z_{k,0}^{b,+})$, $\gamma_2 = (z_{k,0}^{b,-}, +\infty)$ the infinite gaps.

We denote $\Lambda = \Lambda_k^b$ the two-sheeted Riemann surface for each J_k^b , obtained by joining the upper and low rims of two copies of the cut plane $\mathbb{C} \setminus \sigma_{ac}(J_k^{b,0})$ in the usual (crosswise) way. For $j = 0, 1, 2$, we denote the copies of γ_j on Λ^+ (respectively Λ^-) by γ_j^+ (respectively γ_j^-), and put $\gamma_j^c = \overline{\gamma_j^+} \cup \overline{\gamma_j^-}$. By abuse of notation we write also γ_j for $\gamma_j^+ \cup \gamma_j^-$ and for its projection on \mathbb{C} .

If $0 < |c_k| < 1/2$, then $v \in \gamma_1^-$ is an antibound state for J_k^b and if $|c_k| = 1/2$, then $v = z_{k,1}^{b,+}$ or $v = z_{k,1}^{b,-}$ is virtual state (see Definition 1.1 below and Proposition 2.1).

If $c_k = 0$ for some $(k, b) \in \mathbb{Z}_N \times \mathbb{R}$, then (1.8) gives that the spectrum of $J_k^{b,0}$ is pure point:

$$\sigma(J_k^{b,0}) = \sigma_{pp}(J_k^{b,0}) = \{\pm \sqrt{v^2 + 1}\},$$

and each eigenvalue of $J_k^{b,0}$ is a flat band, i.e. has infinite multiplicity.

In [KK2] it is shown that the spectral band $[z_{k,0}^{b,+}, z_{k,1}^{b,-}]$, (respectively $[z_{k,1}^{b,+}, z_{k,0}^{b,-}]$) shrinks to the flat band $-\sqrt{v^2 + 1}$ (respectively $\sqrt{v^2 + 1}$) as $c_k \rightarrow 0$ and the corresponding asymptotics are determined.

Let $b = \pi \left(\frac{1}{2} - \frac{1}{N} \right)$. Then $c_1 = 0$ and $c_k = \cos \pi \left(\frac{1}{2} - \frac{1}{N} + \frac{k}{N} \right)$ and the spectrum of H^b is given by

$$\begin{aligned} \sigma(H^b) &= \sigma_{ac}(H^b) \cup \sigma_{pp}(H^b), & \sigma_{pp}(H^b) &= \{v, \pm \sqrt{1 + v^2}\}, \\ \sigma_{ac}(H^b) &= [z_0^{b,+}, z_0^{b,-}] \setminus \gamma(H^b), & \gamma(H^b) &= (z_1^{b,-}, z_1^{b,+}), \end{aligned} \quad (1.10)$$

where $\gamma(H^b)$ is the gap in the spectrum of H^b . If $b \neq \pi \left(\frac{1}{2} - \frac{1}{N} \right)$ and all $c_k \neq 0$, $k = 1, \dots, N$, then we obtain $\{\pm \sqrt{1 + v^2}\} \notin \sigma_{pp}(H^b)$.

Note that if $c_k = 0$ for some $k \in \mathbb{Z}_N$ then $\sigma_{pp}(H^b) = \{\pm \sqrt{1 + v^2}\} \subset \gamma(H^b)$. From [KK2] we know that $\sigma(H^{b+\frac{\pi}{N}}) = \sigma(H^b)$ for all $b \in \mathbb{R}$. Then we need to consider only the case

$b \in [0, \frac{\pi}{N})$ and in this case we get

$$z_0^{b,+} = \begin{cases} z_{0,0}^{b,+} & \text{if } b \leq \frac{\pi}{2N} \\ z_{N-1,0}^{b,+} & \text{if } b > \frac{\pi}{2N} \end{cases},$$

Moreover, in particular case $\mathcal{B} = 0$, $\frac{N}{3} \in \mathbb{N}$, $b = 0$, we obtain $\gamma(H^0) = (-|v|, |v|)$.

Finitely supported perturbations. We consider the main operator $H^b = H_0^b + V + Q$. Recall that H^b is unitary equivalent to $\oplus_1^N J_k^b$, where $J_k^b = J_k^{b,0} + q$ is given by (1.4) with $q_n = 0$ for $n > p$ and the sequence $y = (y_n)_{n=0}^\infty$ satisfies the Dirichlet boundary condition $y_0 = 0$.

The perturbation q does not change the absolutely continuous spectrum: $\sigma_{ac}(J_k^b) = \sigma_{ac}(J_k^{b,0}) = [\lambda_0^+, \lambda_1^-] \cup [\lambda_1^+, \lambda_0^-]$, where we used the simplified notations $\lambda_0^\pm \equiv z_{k,0}^{b,\pm}$ and $\lambda_1^\pm \equiv z_{k,1}^{b,\pm}$.

In our paper we study the global properties of eigenvalues, virtual states and resonances of $J = J_k^b$. Let $R(\lambda) = (J - \lambda)^{-1}$ denote the resolvent of J and let $\langle \cdot, \cdot \rangle$ denote the scalar product in $\ell^2(\mathbb{N})$. Then for any $f, g \in \ell^2(\mathbb{N})$ the function $\langle Rf, g \rangle$ is defined on Λ_+ outside the poles at the bound states $\lambda_0 \in \gamma_j^+$, $j = 0, 1, 2$. Recall that the bound states are simple. Moreover, if $f, g \in \ell_{\text{comp}}^2(\mathbb{N})$, where $\ell_{\text{comp}}^2(\mathbb{N})$ denotes the ℓ^2 functions on \mathbb{N} with finite support, then the function $\langle Rf, g \rangle$ has an analytic extension from Λ_+ into the Riemann surface Λ .

Definition 1.1. Let $c_k(b) \neq 0$ for some $b \in \mathbb{R}$.

- 1) A number $\lambda_0 \in \Lambda_-$ is a resonance, if the function $\langle Rf, g \rangle$ has a pole at λ_0 for some $f, g \in \ell_{\text{comp}}^2(\mathbb{N})$. The multiplicity of the resonance is the multiplicity of the pole. If $\text{Re } \lambda_0 = 0$, we call λ_0 antibound state.
- 2) A real number $\lambda_0 = \lambda_0^\pm$ or $\lambda_0 = \lambda_1^\pm$ is a virtual state if $\langle Rf, g \rangle$ has a singularity at λ_0 for some $f, g \in \ell_{\text{comp}}^2(\mathbb{N})$.
- 3) The state $\lambda \in \Lambda$ is a bound state or a resonance or a virtual state of J .

We denote the set of all states of J by $\mathfrak{S}(J)$.

In Section 3, 3.2, we give an equivalent characterization of the states.

In the unperturbed case $J^0 = J_k^{b,0}$ we show in Proposition 2.1 that if $0 < c_k \leq 1$, then $\mathfrak{S}(J^0)$ consists of one state: a bound state $v \in \gamma_1^+$, a antibound state $v \in \gamma_1^-$ or a virtual state $v = \lambda_1^\pm$. Note that any such state is projected on the Dirichlet eigenvalue $v \in \mathbb{C}$, $\varphi_2(v) = 0$.

Let ϑ_n, φ_n be the fundamental solutions of the equation $a_{n-1}y_{n-1} + a_n y_{n+1} + v_n y_n = \lambda y_n$, satisfying $\vartheta_0 = \varphi_1 = 1$, $\vartheta_1 = \varphi_0 = 0$. Let f_n^\pm be the Jost solution, $f_n^\pm = \vartheta_n + m_\pm \tilde{\varphi}_n$, where $\tilde{\vartheta}_n, \tilde{\varphi}_n$ denote the solutions to (1.4) satisfying $\tilde{\vartheta}_n = \vartheta_n$, $\tilde{\varphi}_n = \varphi_n$, for $n > p$. Here m_\pm are the Titchmarsh-Weyl functions. The functions φ, ϑ are polynomials, the Jost solutions f^\pm and functions m_\pm are meromorphic functions on Λ . Note that $f^-(\lambda) = \overline{f^+(\bar{\lambda})}$, $\lambda \in \Lambda$, and $f^\pm(\lambda) \in \ell^2(\mathbb{N})$ for any $\lambda \in \Lambda_\pm$. We call f_0^\pm the Jost functions.

We pass to the formulation of main results of the present paper. Recall that all bound and virtual states of $J \equiv J_k^b$ are simple (see Lemma 4.3). In the next theorem we give the characterization of the states of J_k^b .

Theorem 1.1. Let $c_k(b) \neq 0$.

i) The point $\lambda = v \in \gamma_1^+$ or $\lambda = v \in \gamma_1^-$ is a state of $J = J_k^b$ iff the projection of λ on \mathbb{C} is a zero of $\tilde{\varphi}_0$. The value $\lambda \in \Lambda$ whose projection on the complex plane does not coincide with v is a state of J iff $\lambda \in \Lambda$ is a zero of the Jost function f_0^+ :

$$\mathfrak{S}(J) \setminus \{v\} = \{\lambda \in \Lambda : f_0^+(\lambda) = 0\} \subset \left(\bigcup_{j=0,1,2} \overline{\gamma_j^\pm} \right) \cup \Lambda_-.$$

ii) The state $\lambda = \lambda_{0,1}^\pm$ is a virtual state of J iff one of the following two conditions is satisfied:

1) $\lambda \neq v$ and $f_0^+(\lambda) = 0$; 2) $\lambda = v$ and $\tilde{\varphi}_0(\lambda) = 0$.

iii) If $\lambda = v \in \gamma_1^-$ is an antibound state for J then it is necessarily simple.

The distribution of the states is summarized in the following theorem.

Theorem 1.2. Let $c_k(b) \neq 0$, $q_p \neq 0$. Then the Jacobi operator $J \equiv J_k^b$ has $2p$ states counted with multiplicities. Moreover, the following facts hold true.

1) The total number of bound states and virtual states is ≥ 2 .

2) In the closure of the middle gap $\gamma_1^c = \overline{\gamma_1^+} \cup \overline{\gamma_1^-}$ there is always an odd number of states with at least one bound or virtual state.

3) Let $\lambda_1 < \lambda_2$ be any two bound states of J , $\lambda_{1,2} \in \gamma_k^+$, for some $k = 0, 1, 2$, such that there are no other eigenvalues on the interval $\Omega^+ = (\lambda_1, \lambda_2) \subset \gamma_k^+$. Then there exists an odd number ≥ 1 of antibound states on Ω^- , where $\Omega^- \subset \gamma_k^- \subset \Lambda_-$ is the same interval but on the second sheet.

Remarks. 1) If all $c_k \neq 0$ and $q_p \neq 0$, then the operator $\oplus_1^N J_k^b$ has in total $N2p$ states. 2) If p is even and $q_1 = q_3 = \dots = q_{p-1} = 0$, then $\{v\}$ is always a bound state or antibound state (see Lemma 4.5).

In Theorem 1.3 we consider the limit of the states of each J_k^b as $c_k \rightarrow 0$. Recall that operator $J_k^b|_{c_k=0}$ has two flat bands and a finite number of simple eigenvalues.

Theorem 1.3. Let $z_{n,\pm}$, $n \in \mathbb{N}$, be the eigenvalues of the matrix $J_k^b|_{c_k=0}$ given in (1.7). Let $c_k \rightarrow 0 +$.

1) If p is even, then

a) the set of bound states of J_k^b converges to the set $\{z_{n,\pm}, n = 1, \dots, \frac{p}{2}\} \subset \mathbb{R}$,

b) the set of all resonances of J_k^b converges to the set of numbers $\{z_{n,\pm}, n = 1, \dots, \frac{(p-2)}{2}\} \cup \{\mu_{p-1}^0, \mu_p^0\}$, where only the numbers

$$\mu_{p-1,p}^0 = v + \frac{q_{p-1}}{2} \pm \sqrt{\frac{q_{p-1}^2}{4} - \frac{q_{p-1}}{q_p}}, \quad (1.11)$$

can be complex.

2) If p is odd, then

a) the set of bound states of J_k^b converges to the set $\{z_{n,\pm}, n = 1, \dots, \frac{(p+1)}{2}\} \subset \mathbb{R}$;

b) the set of resonances of J_k^b converge to the set of real numbers $\{z_{n,\pm}, n = 1, \dots, \frac{(p-1)}{2}\}$.

In Theorem 1.4 we consider the asymptotics of the states of the half-nanotube Hamiltonian H^b (unitary equivalent to $\oplus_1^N J_k^b$) for large perturbation.

Theorem 1.4. *Suppose $q_j = q_j^0 t$, $j = 1, \dots, p$, where all $q_j^0 \neq 0$ are fixed and $t > 1$. If $\lambda(t) \in \Lambda$ is a state of H^b , then either $|\lambda(t)| \rightarrow \infty$ or $\lambda(t) \rightarrow (-1)^p v$ as $t \rightarrow \infty$.*

If $v \rightarrow \infty$, then (1.9) implies that the absolutely continuous spectrum degenerates into two points $\{v\}$, $\{-v\}$.

Suppose $p = 2$ and $q_1 = 0$ and q_2 is small enough, then the Hamiltonian H^b has precisely $2N$ non-real complex conjugated resonances. More results about the cases $p = 1$ and $p = 2$ are given in Section 5.

The plan of the paper is as follows. In Section 2 we collect some well known facts about the two-periodic Jacobi operators and its perturbations in the form convenient for us.

In Section 3 we describe the properties of the perturbed operator.

In Section 4 we consider the properties of the polynomial $F = \varphi_2 f_0^+ f_0^-$ which plays the crucial role in the proof of the main results, similar to the case [K2]. Theorem 1.2 follows from Lemma 4.2 and Theorem 1.1 follows from Lemmata 4.3 and 4.4. Theorems 1.3 and 1.4 follows from Lemmata 3.1 and 4.1. In Section 5 we consider the cases $p = 1$ and $p = 2$.

2 Periodic Jacobi operator.

In this section we recall some well known facts about the infinite Jacobi matrix \mathbb{J}^0

$$\begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & a & v & 1 & 0 & 0 & \dots \\ \dots & 0 & 1 & -v & a & 0 & \dots \\ \dots & 0 & 0 & a & v & 1 & \dots \\ \dots & 0 & 0 & 0 & 1 & -v & \dots \\ \dots & 0 & 0 & 0 & 0 & a & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}, \quad 0 < a \leq 2 \quad (2.1)$$

and the associated equation for \mathbb{J}^0

$$a_{n-1}y_{n-1} + a_n y_{n+1} + v_n y_n = \lambda y_n, \quad a_{2n+1} = 1, \quad a_{2n} = a, \quad v_{2n+1} = v, \quad v_{2n} = -v, \quad (2.2)$$

$(\lambda, n) \in \mathbb{C} \times \mathbb{Z}$. Introduce fundamental solutions $\varphi = (\varphi_n(z))_{n \in \mathbb{Z}}$ and $\vartheta = (\vartheta_n(z))_{n \in \mathbb{Z}}$ for equation (2.2), under the condition $\vartheta_0 = \varphi_1 = 1$ and $\vartheta_1 = \varphi_0 = 0$. We obtain

$$\begin{aligned} \varphi_0 &= 0, & \varphi_1 &= 1, & \varphi_2 &= \lambda - v, & \varphi_3 &= \frac{\lambda^2 - v^2 - 1}{a}, \\ \vartheta_0 &= 1, & \vartheta_1 &= 0, & \vartheta_2 &= -a, & \vartheta_3 &= -\lambda - v \quad \dots \end{aligned} \quad (2.3)$$

The monodromy matrix M_2 satisfies

$$M_2(\lambda) = \begin{pmatrix} \vartheta_2 & \varphi_2 \\ \vartheta_3 & \varphi_3 \end{pmatrix} = \begin{pmatrix} -a & \lambda - v \\ -\lambda - v & \frac{\lambda^2 - v^2 - 1}{a} \end{pmatrix}. \quad (2.4)$$

The Lyapunov function is defined in the standard way:

$$\Delta = \frac{\text{Tr } M_2}{2} = \frac{\lambda^2 - v^2 - a^2 - 1}{2a} = \cos 2\kappa, \quad (2.5)$$

where κ is the Bloch quasimomentum.

The periodic eigenvalues λ_0^\pm satisfy the equation $\Delta(\lambda) = 1$ and the anti-periodic eigenvalues λ_1^\pm satisfy the equation $\Delta(\lambda) = -1$ and they are given by

$$\lambda_0^\mp = \pm \sqrt{v^2 + (a+1)^2}, \quad \lambda_1^\pm = \pm \sqrt{v^2 + (a-1)^2}. \quad (2.6)$$

The absolutely continuous spectrum of \mathbb{J}^0 has the form

$$\sigma_{\text{ac}}(\mathbb{J}^0) = [\lambda_0^+, \lambda_1^-] \cup [\lambda_1^+, \lambda_0^-] = [\lambda_0^+, \lambda_0^-] \setminus \gamma_1, \quad \gamma_1 = (\lambda_1^-, \lambda_1^+) \quad (2.7)$$

where γ_1 is a gap. Note that $\gamma_1 = (\lambda_1^-, \lambda_1^+) \neq \emptyset$, if $|v| + |a-1| > 0$. We denote also $\gamma_0 = (-\infty, \lambda_0^+)$ and $\gamma_2 = (\lambda_0^-, +\infty)$.

We recall from the Introduction that the two-sheeted Riemann surface Λ is obtained by joining the upper and low rims of two copies Λ^\pm of the cut plane $\mathbb{C} \setminus \sigma_{\text{ac}}(\mathbb{J}^0)$ in the usual (crosswise) way. For $j = 0, 1, 2$, γ_j^+ (respectively γ_j^-) denote the copies of γ_j on Λ^+ (respectively Λ^-), and $\gamma_j^c = \overline{\gamma_j^+} \cup \overline{\gamma_j^-}$. By abuse of notation we write also γ_j for $\gamma_j^+ \cup \gamma_j^-$ and for its projection on \mathbb{C} .

The eigenvalues of M_2 are given by $\xi_\pm^2 = \Delta \pm \sqrt{\Delta^2 - 1}$. On γ_0^+ , we choose

$$\text{for } \lambda \in \gamma_0^+ = (-\infty, \lambda_0^+) \subset \Lambda^+, \quad \xi_+^2 = \Delta - \sqrt{\Delta^2 - 1}, \quad \xi_-^2 = \Delta + \sqrt{\Delta^2 - 1}. \quad (2.8)$$

For others $\lambda \in \Lambda$, the functions $\xi_\pm(\lambda)$ are defined by an analytic continuation.

If $\lambda = \pm v \in \gamma_1^+$ (these numbers will play a special role later) then $\Delta(\pm v) = \frac{-a^2-1}{2a}$ and

$$\xi_+^2(\pm v) = \frac{-a^2-1}{2a} + \left| \frac{a^2-1}{2a} \right| = \begin{cases} -a & \text{if } 0 < a < 1, \\ -1/a & \text{if } a > 1, \end{cases} \quad (2.9)$$

and opposite for $\xi_-^2(\pm v)$.

Then for $\lambda \in \gamma_0 \cup \gamma_1 \cup \gamma_2$ we have $|\xi_+^2| < 1$ and $|\xi_-^2| > 1$. The eigenvectors of M_2 are chosen in the form $(1, m_\pm)$ and then the Titchmarsh-Weyl functions are

$$m_\pm(\lambda) = \frac{\xi_\pm^2 - \vartheta_2}{\varphi_2} = \frac{\xi_\pm^2 + a}{\lambda - v}. \quad (2.10)$$

For $\lambda \in \gamma_1^+$ we have also

$$m_\pm = \frac{\phi \pm \sqrt{\Delta^2 - 1}}{\varphi_2} = \frac{\Delta + a \pm \sqrt{\Delta^2(\lambda) - 1}}{\lambda - v} = \frac{\phi \pm i \sin 2\kappa}{\lambda - v} \quad (2.11)$$

$$\phi = \frac{\varphi_3 - \vartheta_2}{2} = \frac{\lambda^2 - v^2 + a^2 - 1}{2a} = \Delta + a. \quad (2.12)$$

On each γ_k^+ , $k = 0, 1, 2$, the quasimomentum $\varkappa(\lambda)$ has constant positive imaginary part and we put $\varkappa = ih$, $h = h_k > 0$. Then $\Delta = \cosh(2h)$ and

$$i \sin 2\varkappa = -(-1)^k \sqrt{\Delta^2(\lambda) - 1} = -(-1)^k \sinh 2h. \quad (2.13)$$

Now the Floquet solutions $\psi_n^\pm = \vartheta_n + m_\pm \varphi_n$ are

$$\psi_0^\pm = 1, \quad \psi_1^\pm = m_\pm, \quad \psi_2^\pm = e^{\pm 2i\varkappa} = \xi_\pm^2, \quad \psi_{2n}^\pm = \xi_\pm^{2n}, \quad \psi_{2n+1}^\pm = \xi_\pm^{2n} m_\pm, \quad (2.14)$$

where $\xi_\pm^2 = e^{\pm 2i\varkappa}$ are the Floquet multipliers. Recall that $\psi_n^\pm \in \ell^2(\mathbb{N})$ for any $\lambda \in \Lambda^\pm$.

Note the following simple identities which will be used in the paper:

$$\phi^2 + 1 - \Delta^2 = 1 - \varphi_3 \vartheta_2 = -\vartheta_3 \varphi_2. \quad (2.15)$$

Let $\{\phi_n, \psi_n\} = a_n(\phi_n \psi_{n+1} - \phi_{n+1} \psi_n)$ denote the Wronskian.

In the next theorem we describe the states of the restriction of J^0 to \mathbb{N} defined in (1.4) with $\tilde{v}_n = v_n$.

Proposition 2.1 (Unperturbed case). *The half-periodic Jacobi operator J^0 given by equation (1.4) with $\tilde{v}_n = v_n$, has absolutely continuous spectrum (2.7): $\sigma_{ac}(J^0) = [\lambda_0^+, \lambda_1^-] \cup [\lambda_1^+, \lambda_0^-]$ and a state at $\lambda = v \in \overline{\gamma_1^+} \cup \overline{\gamma_1^-}$, whose projection $v \in \mathbb{C}$ satisfies $\varphi_2(v) = 0$. There are three possibilities:*

if $a > 1$ then J^0 has simple bound state at $\lambda = v \in \gamma_1^+$;

if $0 < a < 1$ then J^0 has simple antibound state at $\lambda = v \in \gamma_1^-$;

if $a = 1$ then $\lambda = v$ is a simple virtual state, $v = \lambda_1^+$ or $v = \lambda_1^-$ if $v > 0$ respectively $v < 0$.

Proof: The kernel of the resolvent of J^0 is given by

$$R_0(n, m) = -\frac{\varphi_n \psi_m^+}{\{\varphi, \psi^+\}}, \quad n < m,$$

where $\{\varphi, \psi^+\} = -a$. According to Lemma 3.2 (see Section 3), the bound states (resonances) are the poles of $\mathcal{R}_0(n) = \psi_n^+(\lambda) = \vartheta_n(\lambda) + m_+(\lambda) \varphi_n(\lambda)$ on Λ_+ (respectively on Λ_-). Hence, the only state is the pole of m_+ on Λ_\pm , whose projection on \mathbb{C} is the zero of $\varphi_2(\lambda)$, i.e. $\lambda = v \in \gamma_1$.

We have

$$m_+ = \frac{\xi_+^2 + a}{\lambda - v}, \quad a = 2|c_k|, \quad c_k = \cos\left(b + \frac{\pi k}{N}\right).$$

If $0 < a < 1$, then by (2.9) $\lambda = v \in \gamma_1^+$ is a simple zero for the numerator while at $\lambda = v \in \gamma_1^-$ the numerator is non-zero. Thus $\lambda = v$ is an antibound state. Similar we get that if $1 < a < 2$, then $\lambda = v$ is a bound state.

If $a = 1$ then $\Delta = (\lambda^2 - v^2 - 2)/2$ and

$$\Delta^2 - 1 = -(\lambda - v)(\lambda + v) + \frac{(\lambda - v)^2(\lambda + v)^2}{4}.$$

Suppose $v > 0$, then $v = \lambda_1^+$. Let $\lambda - v = -\epsilon$, $\epsilon > 0$, and let $\epsilon \rightarrow 0$. Then

$$\Delta = -1 - v\epsilon + \mathcal{O}(\epsilon^2), \quad \sqrt{\Delta^2 - 1} = \sqrt{\epsilon}\sqrt{2v} + \mathcal{O}(\epsilon),$$

and

$$m_+(v - \epsilon) = \frac{\Delta + a + \sqrt{\Delta^2 - 1}}{\lambda - v} = \frac{\sqrt{\epsilon}\sqrt{2v} + \mathcal{O}(\epsilon)}{\epsilon} = \frac{\sqrt{2v}}{\sqrt{\epsilon}} + \mathcal{O}(1). \quad (2.16)$$

Thus if $a = 1$, the function $(\mathcal{R}_n(\lambda))^2$ has a pole at $\lambda = v$ and $\lambda = v$ is a virtual state. \square

3 Jost functions

We introduce the Jost solutions as solutions f_n^\pm , of the equation

$$a_{n-1}y_{n-1} + a_n y_{n+1} + \tilde{v}_n y_n = \lambda y_n, \quad n \in \mathbb{N}, \quad \lambda \in \Lambda, \quad (3.1)$$

satisfying

$$f_n^\pm = \psi_n^\pm, \quad \text{for } n > p, \quad (3.2)$$

where ψ_n^\pm are the Floquet solutions (2.14) for the unperturbed problem, and $\tilde{v}_j = v_j + q_j$ with $q_n = 0$ for $n > p$. We recall that, as in (2.2), we have $v_{2n+1} = -v_{2n} = v \in \mathbb{R}$, $a_{2n+1} = 1$, $a_{2n} = a = 2|c_k| \neq 0$, $c_k = \cos(b + \frac{\pi k}{N})$. We have $\overline{f_n^\pm}(\bar{\lambda}) = f_n^\mp(\lambda)$, $\lambda \in \Lambda$.

The equation (3.1) has unique solutions $\tilde{\vartheta}_n$, $\tilde{\varphi}_n$ such that

$$\tilde{\vartheta}_n(\lambda) = \vartheta_n(\lambda), \quad \tilde{\varphi}_n(\lambda) = \varphi_n(\lambda) \quad \text{for } n > p, \quad \lambda \in \mathbb{C}.$$

The functions $\tilde{\vartheta}_n(\cdot)$, $\tilde{\varphi}_n(\cdot)$ are polynomials. The functions f_n^\pm have the form

$$f_n^\pm = \tilde{\vartheta}_n + m_\pm \tilde{\varphi}_n, \quad m_\pm = \frac{\phi \pm i \sin 2\kappa}{\varphi_2} = \frac{\Delta + a \pm \sqrt{\Delta^2(\lambda) - 1}}{\lambda - v}. \quad (3.3)$$

Here ϕ is defined in (2.12), $\varphi_2 = \lambda - v$ and Δ is the Lyapunov function. The functions f_0^\pm are called Jost functions. The Jost functions are analytic at all $\lambda \in \Lambda$ whose projection on the complex plane \mathbb{C} is different from v , and has branch points $\lambda_{0,1}^\pm$.

The asymptotics of the Jost functions are given in the following Lemma.

Lemma 3.1. *Let $p, n \in \mathbb{N}$ and $p \geq n$. Suppose $q_p \neq 0$.*

1) *If p is even ($a_p = a$, $v_p = -v$), then*

for $\lambda \in \gamma_{0,2}^+$ in the limit $|\lambda| \rightarrow \infty$, we have

$$f_0^+ = 1 - \lambda^{-1} \sum_{k=1}^p q_k + \mathcal{O}(\lambda^{-2}), \quad f_0^- = \frac{\lambda^{2p-1}}{a^p} [-q_p + \mathcal{O}(\lambda^{-1})];$$

for $\lambda \in \gamma_1^+$ as $a \rightarrow 0+$, we have

$$\begin{aligned} f_0^+ &= (2\delta)^{-p/2} \prod_{k=1}^{p-1} \left[(\lambda - \tilde{v}_k)(\lambda - \tilde{v}_{k+1}) - 1 \right] + \delta^{-p/2} \mathcal{O}(a^2), \\ f_0^- &= \frac{(2\delta)^{p/2}}{a^p} \left[(\lambda - \tilde{v}_{p-1}) \left\{ (\lambda - \tilde{v}_p) - \frac{2\delta}{\lambda - v} \right\} - 1 \right] \prod_{k=1}^{p-3} \left[(\lambda - \tilde{v}_k)(\lambda - \tilde{v}_{k+1}) - 1 \right] \\ &\quad + \delta^{p/2} \mathcal{O}(a^2), \end{aligned} \quad (3.4)$$

where $\delta = (\lambda^2 - v^2 - 1)/2$;

if $q_k = tq_k^0$ with all $q_k^0 \neq 0$ and $t \rightarrow \infty$, then we have $f_0^+ = t^p \frac{\xi_+^p}{a^{p/2}} \prod_{k=1}^p q_k^0 + \mathcal{O}(t^{p-1})$.

2) If p is odd ($a_p = 1$, $v_p = v$), then

for $\lambda \in \gamma_{0,2}^+$ in the limit $|\lambda| \rightarrow \infty$, we have

$$f_0^+ = 1 - \lambda^{-1} \sum_{k=1}^p q_k + \mathcal{O}(\lambda^{-2}), \quad f_0^- = \frac{\lambda^{2p-1}}{a^{p+1}} [-q_p + \mathcal{O}(\lambda^{-1})]; \quad (3.5)$$

for $\lambda \in \gamma_1^+$, as $a \rightarrow 0+$, we have

$$\begin{aligned} f_0^+ &= (2\delta)^{-(p+1)/2} [(\lambda - \tilde{v}_p)(\lambda + v) - 1] \prod_{k=1}^{p-2} [(\lambda - \tilde{v}_k)(\lambda - \tilde{v}_{k+1}) - 1] + \delta^{-(p+1)/2} \mathcal{O}(a^2), \\ f_0^- &= \frac{(2\delta)^{(p+1)/2}}{a^{p+1}} \cdot \frac{-q_p}{\lambda - v} \prod_{k=1}^{p-2} [(\lambda - \tilde{v}_k)(\lambda - \tilde{v}_{k+1}) - 1] + \delta^{(p+1)/2} \mathcal{O}(a^2), \end{aligned}$$

if $q_k = tq_k^0$ with $q_k^0 \neq 0$ and $t \rightarrow \infty$, then $f_0^+ = t^p \frac{\xi_+^p}{a^{(p+1)/2}} \frac{1 + a\xi_-^2}{\lambda - v} \prod_{k=1}^p q_k^0 + \mathcal{O}(t^{p-1})$.

The proof is technical and uses the standard arguments. The asymptotics of f_0^+ on $\gamma_{0,2}^+$ as $\lambda \rightarrow \infty$ are well known (see for example Teschl [T]).

It is well known that the spectrum of $J = J_k^b$, introduced in (1.4), consists of absolutely continuous part $\sigma_{ac}(J) = \sigma_{ac}(J^0)$ and a finite number of simple bound states in each gap γ_k^+ , $k = 0, 1, 2$. The states of J correspond to the poles of a meromorphic function: resolvent or its square.

The kernel of the resolvent of J is

$$R(n, m) = \langle e_n, (J - \lambda)^{-1} e_m \rangle = -\frac{\Phi_n f_m^+}{\{\Phi, f^+\}}, \quad n < m,$$

where $e_n = (\delta_{n,j})_{j \in \mathbb{N}}$, $J\Phi_n = \lambda\Phi_n$, $\Phi_0 = 0$, $\Phi_1 = 1$, and the Wronskian $\{\Phi, f^+\} = -a_0 f_0^+$.

Each function $\Phi_n(\lambda)$, $n \in \mathbb{N}$, is polynomial in λ . The function $R(n, m)$ is meromorphic on Λ for each $n, m \in \mathbb{Z}$. The singularities of $R(n, m)$ are given by the singularities of

$$\mathcal{R}_n(\lambda) = \frac{f_n^+(\lambda)}{f_0^+(\lambda)} = \frac{\tilde{\vartheta}_n(\lambda) + m_+(\lambda)\tilde{\varphi}_n(\lambda)}{f_0^+(\lambda)}.$$

The following Lemma follows from Definition 1.1.

Lemma 3.2. 1) A real number $\lambda_0 \in \gamma_j^+$, $j = 0, 1, 2$, is a bound state, if the function $\mathcal{R}_n(\lambda)$ has a pole at λ_0 for almost all $n \in \mathbb{N}$ (eventually except a finite number of n 's) (it is known that the bound states are simple).

2) A number $\lambda_0 \in \Lambda_-$, is a resonance, if the function $\mathcal{R}_n(\lambda)$ has a pole at λ_0 for almost all $n \in \mathbb{N}$ (eventually except a finite number of n 's). The multiplicity of the resonance is the multiplicity of the pole. If $\operatorname{Re} \lambda_0 = 0$, we call λ_0 antibound state.

3) A real number $\lambda_0 = \lambda_0^\pm$ or $\lambda_0 = \lambda_1^\pm$ is a virtual state if $(\mathcal{R}_n(\lambda))^2$ or $\mathcal{R}_n(\lambda)$ has a pole at λ_0 for almost all $n \in \mathbb{N}$ (eventually except a finite number of n 's).

4) The state $\lambda \in \Lambda$ is a bound state, resonance or virtual state.

We recall that the set of all states of J is denoted by $\mathfrak{S}(J)$.

Each function $f_n^+(\lambda)$, $n \in \mathbb{N}$, is analytic at all $\lambda \in \Lambda$ whose projection on the complex plane \mathbb{C} is different from v . The Jost function $f_0^+(\lambda)$ has finite number of real zeros on each γ_k^\pm and finite number of complex conjugated zeros on Λ_- .

Remark that if $\lambda_0 \in \gamma_k$, for some $k = 0, 1, 2$ (then $\lambda_0 \neq \lambda_{0,1}^\pm$), and if $f_0^+(\lambda_0) \neq 0$ and $\varphi_2(\lambda_0) \neq 0$, then the resolvent is analytic at λ_0 .

As $\vartheta_n(\lambda)$, $\tilde{\varphi}_n(\lambda)$ are polynomials then the singularities are zeros of $f_0^+(\lambda)$ and eventually singularities of m_+ at $\lambda = v$ (as in the unperturbed case).

To describe the states of the general operator J stated in Theorem 1.2, it is convenient to introduce a special polynomial whose zeros give all states of J .

4 Function F and proofs of main results

We introduce function $F(\lambda) = \varphi_2 f_0^+ f_0^-$.

Lemma 4.1. Suppose $q_p \neq 0$.

i) The function $F(\lambda) = \varphi_2 f_0^+ f_0^-(\lambda)$ is polynomial of degree $2p$ and satisfies

$$F = \varphi_2 \tilde{\vartheta}_0^2 + 2\phi \tilde{\vartheta}_0 \tilde{\varphi}_0 - \vartheta_3 \tilde{\varphi}_0^2 = (\lambda - v) \tilde{\vartheta}_0^2 + \frac{1}{a} (\lambda^2 - v^2 + a^2 - 1) \tilde{\vartheta}_0 \tilde{\varphi}_0 + (\lambda + v) \tilde{\varphi}_0^2. \quad (4.1)$$

ii) For $\lambda \in \mathbb{C}$, in the limit $|\lambda| \rightarrow \infty$, we have asymptotics

$$F = \frac{\lambda^{2p}}{(a_p \dots a_0)^2} [-a^2 q_p + \mathcal{O}(|\lambda|^{-1})], \quad \text{if } p \text{ is even}, \quad (4.2)$$

$$F = \frac{\lambda^{2p}}{(a_p \dots a_0)^2} [-q_p + \mathcal{O}(|\lambda|^{-1})], \quad \text{if } p \text{ is odd}, \quad (4.3)$$

where $\mathcal{O}(|\lambda|^{-1})$ is uniformly bounded in a . In particular, if $\lambda \in \mathbb{R}$ and $|\lambda| \rightarrow \infty$, we have $\text{sign}(F) = -\text{sign}(q_p)$.

iii) In the limit $a \rightarrow 0$, the function F behaves as follows:
if p is even, then

$$F = \frac{1}{a^p} [(\lambda - \tilde{v}_{p-1})(\lambda - \tilde{v}_p) - 1] [(\lambda - \tilde{v}_{p-1})(1 - q_p(\lambda - v)) - (\lambda - v)] \quad (4.4)$$

$$\cdot \prod_{k=1}^{p-3} [(\lambda - \tilde{v}_k)(\lambda - \tilde{v}_{k+1}) - 1]^2 + \mathcal{O}(a^{2-p}), \quad (4.5)$$

if p is odd

$$F = \frac{-q_p}{a^{p+1}} [(\lambda - \tilde{v}_p)(\lambda + v) - 1] \prod_{k=1}^{p-2} [(\lambda - \tilde{v}_k)(\lambda - \tilde{v}_{k+1}) - 1]^2 + \mathcal{O}(a^{1-p}).$$

Here $\mathcal{O}(a^j)$ is uniformly bounded in $\lambda \in \mathbb{C}$.

iv) Put $q_j = tq_j^0$ for all $q_j^0 \neq 0$ fixed and $t \rightarrow \infty$. Then,

$$F(\lambda) = t^{2p} \frac{(\lambda - v)}{a^p} \left[\prod_{k=1}^p (q_p^0)^2 + \mathcal{O}(t^{2p-1}) \right], \quad \text{if } p \text{ is even}$$

$$F(\lambda) = t^{2p} \frac{(\lambda + v)}{a^{p+1}} \left[\prod_{k=1}^p (q_p^0)^2 + \mathcal{O}(t^{2p-1}) \right], \quad \text{if } p \text{ is odd},$$

uniformly bounded in $\lambda \in \mathbb{C}$.

Proof: We have

$$\begin{aligned} f_0^+ f_0^- &= (\tilde{\vartheta}_0 + m_+ \tilde{\varphi}_0)(\tilde{\vartheta}_0 + m_- \tilde{\varphi}_0) = \tilde{\vartheta}_0^2 + (m_+ + m_-) \tilde{\vartheta}_0 \tilde{\varphi}_0 + m_+ m_- \tilde{\varphi}_0^2 \\ &= \tilde{\vartheta}_0^2 + \frac{2\phi}{\varphi_2} \tilde{\vartheta}_0 \tilde{\varphi}_0 + \frac{\phi^2 + 1 - \Delta^2}{\varphi_2^2} \tilde{\varphi}_0^2 = \tilde{\vartheta}_0^2 + \frac{2\phi}{\varphi_2} \tilde{\vartheta}_0 \tilde{\varphi}_0 + \frac{-\vartheta_3 \varphi_2}{\varphi_2^2} \tilde{\varphi}_0^2 \\ &= \tilde{\vartheta}_0^2 + \frac{2\phi}{\varphi_2} \tilde{\vartheta}_0 \tilde{\varphi}_0 - \frac{\vartheta_3}{\varphi_2} \tilde{\varphi}_0^2, \end{aligned}$$

where we have used (2.11) and (2.15). The degree $2p$ will come from $\varphi_2 = \lambda - v$ and asymptotics (4.2), (4.3).

Now as F is polynomial, in order to prove the asymptotics $|\lambda| \rightarrow \infty$ on \mathbb{C} it is enough to consider $\lambda \rightarrow +\infty$ on γ_2^+ , $a \rightarrow 0$ or $q_j \rightarrow \infty$ for $\lambda \in \gamma_1^+$. The proof thus follows from the asymptotics of the Jost functions given in Lemma 3.1. \square

From iii), Lemma 4.1, we get the leading orders of the zeros of F as $a \rightarrow 0$ which correspond to the leading orders of the states. Using Lemma 3.1 we know if the limiting state is a bound state or a resonance. Recall the eigenvalues of the matrix (1.7) given by

$z_{n,\pm} = v_n^+ \pm |v_n^{-2} + 1|^{\frac{1}{2}}$ (see (1.8)). If $q_p \neq 0$ and if p is even, then there are at most p eigenvalues $z_{n,\pm}$, $n = 1, 2, \dots, \frac{p}{2}$, where

$$v_n^+ = \frac{\tilde{v}_{2n-1} + \tilde{v}_{2n}}{2} = \frac{q_{2n-1} + q_{2n}}{2}, \quad v_n^- = \frac{\tilde{v}_{2n-1} - \tilde{v}_{2n}}{2} = v + \frac{q_{2n-1} - q_{2n}}{2},$$

if p is odd, then there are at most $p + 1$ eigenvalues $z_{n,\pm}$, $n = 1, 2, \dots, \frac{(p-1)}{2}$, where

$$v_n^+ = \frac{\tilde{v}_{2n-1} + \tilde{v}_{2n}}{2} = \frac{q_{2n-1} + q_{2n}}{2}, \quad v_n^- = \frac{\tilde{v}_{2n-1} - \tilde{v}_{2n}}{2} = v + \frac{q_{2n-1} - q_{2n}}{2},$$

$$v_{(p+1)/2}^+ = \frac{\tilde{v}_p - v}{2} = \frac{q_p}{2}, \quad v_{(p+1)/2}^- = \frac{\tilde{v}_p + v}{2} = v + \frac{q_p}{2}.$$

Recall that, as perturbations have finite support, then there are also two flat bands (two eigenvalues with infinite multiplicities) given by $z_{n,\pm} = \pm |v^2 + 1|^{\frac{1}{2}}$, where $n \geq \frac{p}{2} + 1$ if p is even or $n \geq \frac{(p+1)}{2} + 1$ if p is odd. Similar, using Lemma 3.1, we get the leading orders of the resonances. In the even case the resonances can converge to complex number - zeros of the factor $(\lambda - \tilde{v}_{p-1}) \{(\lambda - \tilde{v}_p) - \frac{2\delta}{\lambda - v}\} - 1$ in (3.4) or equivalently zeros of the polynomial $(\lambda - \tilde{v}_{p-1})(1 - q_p(\lambda - v)) - (\lambda - v)$ (see (4.4)).

This implies Theorem 1.3.

Theorem 1.4 follows from 3.1 and iv) in Lemma 4.1.

In the next Lemma we state the crucial properties of the function F .

Lemma 4.2. *i) Suppose that $\lambda_1 \in \gamma_k^+$, for $k = 0, 1$ or 2 , and either*

- a) $f_0^+(\lambda_1) = 0$, i.e. λ_1 is an eigenvalue of J with the eigenfunction $y_n = f_n^+(\lambda_1)$, or*
- b) $\lambda_1 = v$. Let λ_1 also denote the projection of $\lambda_1 \in \gamma_k^+$ on \mathbb{C} .*

Then $(-1)^k \dot{F}(\lambda_1) < 0$ and function F has simple zeros at all bound states of J . Moreover if $\lambda_1 = v$, then $\tilde{\varphi}_0(v) = 0$, $f_0^+(\lambda)$ is analytic at $\lambda = v \in \gamma_1^+$ and $f_0^+ \neq 0$.

ii) We have $F(\lambda) =$

$$\varphi_2 \left(\tilde{\vartheta}_0 + \frac{\phi}{\varphi_2} \tilde{\varphi}_0 \right)^2 + \frac{1 - \Delta^2}{\varphi_2} \tilde{\varphi}_0^2 = \varphi_2 \left(\tilde{\vartheta}_0 + \frac{\phi}{\varphi_2} \tilde{\varphi}_0 \right)^2 + \frac{-(\lambda^2 - \lambda_0^2)(\lambda^2 - \lambda_1^2)}{4a^2 \varphi_2} \tilde{\varphi}_0^2, \quad (4.6)$$

where $\lambda_0 = \lambda_0^\mp$ and $\lambda_1 = \lambda_1^\pm$ are the endpoints of $\sigma_{ac}(J^0) = [\lambda_0^+, \lambda_1^-] \cup [\lambda_1^+, \lambda_0^-]$.

We have $F(\lambda) < 0$, for $\lambda \in (\lambda_0^+, \lambda_1^-)$, and $F(\lambda) > 0$, for $\lambda \in (\lambda_1^+, \lambda_0^-)$.

Remarks. 1) Lemma 4.2 (with proper modifications) is also true for general Jacobi operators on the half-line and is proven in paper [IK3]. The methods remind the approach of [K2] to the periodic Schrödinger operator plus compactly supported potentials on the half-line.

2) It follows that $F(\lambda)$, which is real on the real axis, is decreasing function at any eigenvalue $\lambda_1 \in \gamma_{0,2}^+$, and increasing function at any eigenvalue $\lambda_1 \in \gamma_1^+$.

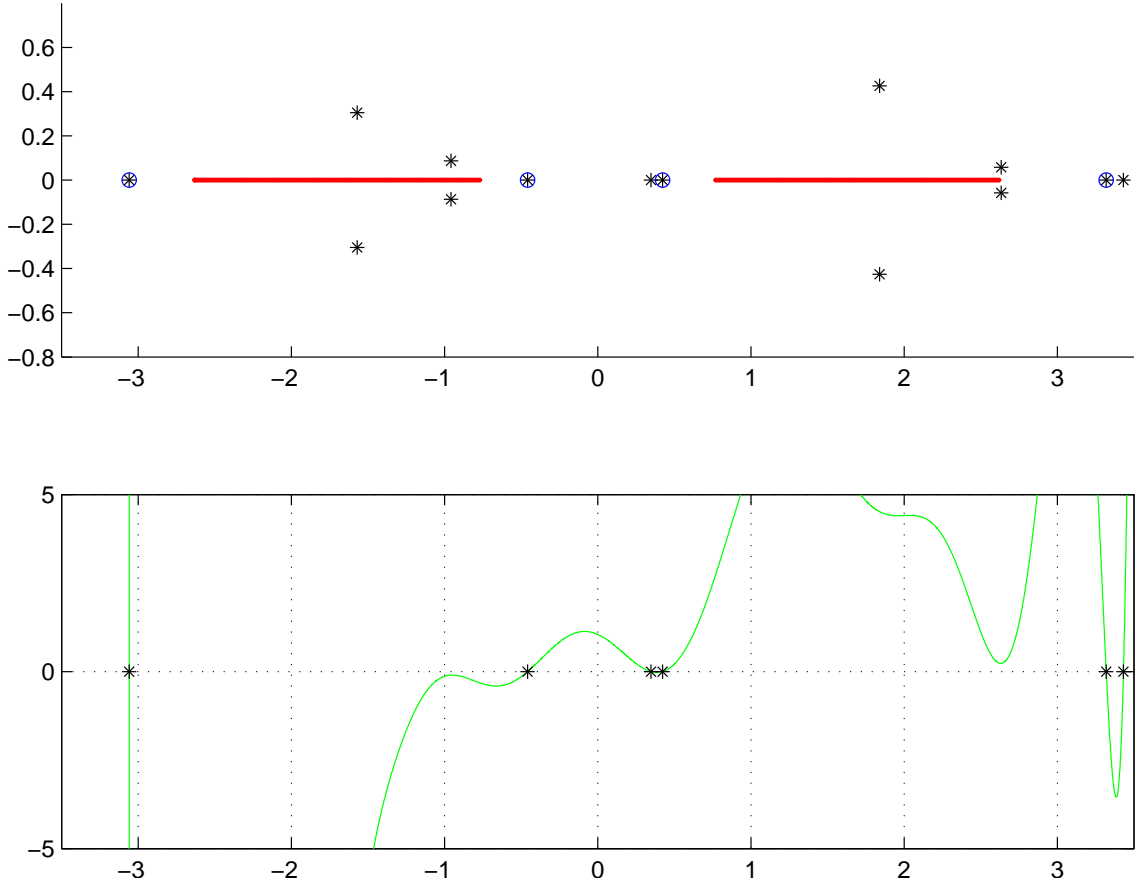


Figure 1: Function F and the states, the bound states are encircled.

It follows that all bound states of J are simple and that for any two eigenvalues $\lambda_{1,2} \in \gamma_k^+$ such that the interval $\Omega^+ = (\lambda_1, \lambda_2) \subset \gamma_k^+$ does not contain any other bound states there is an odd number of antibound states λ_0 in the same interval $\Omega^- \subset \gamma_k^- \subset \Lambda_-$ on the second sheet, and $(-1)^k \dot{F}(\lambda_0) > 0$.

3) From ii) it follows that there is always at least one eigenvalue in the middle gap γ_1 or a virtual state at λ_1^\pm . Moreover, using that from Lemma 4.1 it follows that function F has the same sign when $\lambda \rightarrow \pm\infty$, we get that

if $\text{sign}(F)(\pm\infty) < 0$, then there are at least two eigenvalues: one in γ_1 another in γ_2 (which can become virtual states); if $\text{sign}(F)(\pm\infty) > 0$ and $0 < a < 1$, then there are at least two eigenvalues: one in γ_0 , another in γ_1 (which can become virtual states).

Now the proof of Theorem 1.1 follows from the following two Lemmata which are proved in [IK3] in the general case.

Lemma 4.3 (Virtual states). *Let λ_0 denote any of $\lambda_{0,1}^\pm$ and let $\lambda = \lambda_0 + \epsilon$ for $\epsilon > 0$ small enough.*

i) If $\lambda, \lambda_0 \neq v$ and $f_0^+(\lambda_0) = 0$, then λ_0 is a simple zero of F , λ_0 is a virtual state of J , and

$$f_0^+(\lambda) = \tilde{\varphi}_0(\lambda_0)c\sqrt{\epsilon} + \mathcal{O}(\epsilon), \quad \mathcal{R}_n(\lambda) = \frac{f_n^+(\lambda)}{\tilde{\varphi}_0(\lambda_0)c\sqrt{\epsilon}}(1 + \mathcal{O}(\sqrt{\epsilon})), \quad c\tilde{\varphi}_0(\lambda_0) \neq 0. \quad (4.7)$$

ii) If $\lambda_0 = v$ (which happens if $a = 1$) and $\tilde{\varphi}_0(\lambda_0) \neq 0$, then $F(\lambda_0) \neq 0$ and each $\mathcal{R}_n(\cdot)$, $n \in \mathbb{N}$, does not have singularity at λ_0 and λ_0 is not a virtual state of J .

iii) If $\lambda_0 = v$ and $\tilde{\varphi}_0(\lambda_0) = 0$, then λ_0 is a virtual state of J , $f_0^\pm(\lambda_0) \neq 0$, λ_0 is simple zero of F , and each $(\mathcal{R}_n(\cdot))^2$, $n \in \mathbb{N}$, has pole at λ_0 .

Lemma 4.4. *The projection $\pi : \Lambda \mapsto \mathbb{C}$ of the set of states of J on Λ coincides with the set of zeros of F on the complex plane \mathbb{C} :*

$$\pi\mathfrak{S}(J) = \text{Zeros}(F).$$

Moreover, the multiplicities of bound states and resonances are equal to the multiplicities of zeros of F . All bound states are simple.

Suppose $\lambda_0 = \lambda_0^\pm$ or $\lambda_0 = \lambda_1^\pm$ and $\tilde{\varphi}_0(\lambda_0) \neq 0$. Then λ_0 is a virtual state iff $F(\lambda)$ has zero at λ_0 . It will be automatically simple.

In the next Lemma we consider a special case when we have a simple criterium when $\lambda = v$ is a state.

Lemma 4.5. *Suppose that p is even and for any $n \in \mathbb{N}$, $\tilde{v}_{2n+1} = v_{2n+1} = v$.*

Then $\tilde{\varphi}_0(v) = 0$ and $F(v) = 0$. Thus $\lambda = v$ is a state.

Proof: From the well known explicit formula $\varphi_{2n} = (\lambda - v) \sin n2\kappa / \sin 2\kappa$ it follows that $\varphi_{2n}(v) = 0$ for any $n \in \mathbb{N}$. From the equation $Jy = \lambda y$ we have the iteration formula:

$$\tilde{\varphi}_{2n} = \frac{(\lambda - \tilde{v}_{2n+1})\tilde{\varphi}_{2n+1} - \tilde{\varphi}_{2n+2}}{a}. \quad (4.8)$$

But $\tilde{\varphi}_k = \varphi_k$ for $k \geq p+1$ and $\tilde{v}_{2n+1} = v$. Thus, starting with $2n = p$ and iterating (4.8), we get $\tilde{\varphi}_{2n}(v) = 0$, $\tilde{\varphi}_{2n-2}(v) = 0$, \dots , $\tilde{\varphi}_0(v) = 0$: all functions $\tilde{\varphi}_k$ with even indexes are zeros at $\lambda = v$. Then from (4.1) it follows that $F(v) = 0$. \square

5 Examples $p = 1$ and $p = 2$.

In this Section we consider the special cases $p = 1$ and $p = 2$ when the properties of the states can be analyzed in more details. Using that

$$f_p^+ = \frac{(\lambda - \tilde{v}_{p+1})f_{p+1}^+ - a_{p+1}f_{p+2}^+}{a_p} = \frac{\xi_+^{p+1}}{a_p}((\lambda + v) - am_+) = \frac{\xi_+^{p+1}}{a_p} \frac{1 + a\xi_-^2}{\lambda - v},$$

$$f_{p-1}^+ = \frac{(\lambda - \tilde{v}_p)f_p^+ - a_p f_{p+1}^+}{a_{p-1}} = \frac{\xi_-^{p+1}}{a_p a_{p-1}} \left((\lambda - \tilde{v}_p) \frac{1 + a\xi_-^2}{\lambda - v} - a_p^2 \right),$$

and $\varphi_2 = \lambda - v$, $\xi_+^2 \xi_-^2 = 1$, $\xi_+^2 + \xi_-^2 = 2\Delta = (\lambda^2 - v^2 - a^2 - 1)/a \Rightarrow 2a\Delta + 1 + a^2 = \lambda^2 - v^2$, we get for $p = 1$, $a_0 = a$, $a_1 = 1$, $v_1 = v + q_1$,

$$F(\lambda) = \varphi_2 f_0^+ f_0^- = a^{-2} \left(-q_1 \lambda^2 + \lambda [q_1^2 + a^2] + (q_1^2 v + q_1(v^2 + 1 - a) - va^2) \right),$$

If $v = v_1$ (the unperturbed case) then $F = a^2(\lambda - v)$ and $\lambda = v$ is the only state, see Lemma 2.1. The discriminant of the quadratic equation is

$$D = (a^2 - (v_1^2 - v^2))^2 + 4(v_1 - v)^2 = (q_1^2 + 2vq_1 - a^2)^2 + 4q_1^2 > 0 \text{ if } v_1 \neq v.$$

Thus we get that the states are real. By Lemma 4.2 on F , part ii), both states are bound states: no resonances for $p = 1$. One can check directly that if perturbation is non-trivial ($v \neq v_1$) then there are no virtual states if $p = 1$: if $\lambda_0 = \lambda_0^\pm$ is virtual state then $\xi_-^2 = \Delta(\lambda_0) = \pm 1$, and

$$f_0^+(\lambda_0) = \frac{\pm 1}{a} \left((\lambda - v_1) \frac{1 \pm a}{\lambda - v} - 1 \right) = 0 \Leftrightarrow (\lambda_0 - v_1)(1 \pm a) = \lambda_0 - v, \quad \lambda_0 \neq v,$$

which never happens. Thus we have

Proposition 5.1. *For $p = 1$, $v \neq v_1$, J has two real bound states:*

$$\lambda_{\pm} = \frac{[q_1^2 + a^2] \pm \sqrt{(q_1^2 + 2vq_1 - a^2)^2 + 4q_1^2}}{2q_1} = \frac{q_1}{2} + \frac{a^2}{2q_1} \pm \sqrt{\left(\frac{q_1}{2} + v - \frac{a^2}{2q_1} \right)^2 + 1}.$$

In the limit $a \rightarrow 0$, we get straightforward $\lambda_{1,2} = \frac{1}{2}(q_1 \pm \sqrt{(2v + q_1)^2 + 4}) + \mathcal{O}(a^2)$. As $v \rightarrow \infty$, we have $\lambda_{1,2} \sim \pm v \rightarrow \pm \infty$. As $v \rightarrow 0$, we have $\lambda_{1,2} \rightarrow (2q_1)^{-1}([q_1^2 + a^2] \pm \sqrt{(q_1^2 - a^2)^2 + 4q_1^2})$. Next we get:

if $q_1 \rightarrow 0$, then $\lambda_+ \sim a^2/q_1 \rightarrow \infty$, and $\lambda_- \rightarrow v$;

if $q_1 \rightarrow \infty$, we have $\lambda_+ \sim q_1 \rightarrow \infty$, and $\lambda_- \rightarrow -v$.

Now we consider in detail the properties of the states in the simplest non-trivial case $p = 2$, which allows the complex resonances. Let $D(p_3)$ denote the generalized discriminant of a special cubic polynomial which will be explained below and given by the following cumbersome formula:

$$\begin{aligned} D(p_3) = & (vq_2 + q_2^2)^2 q_2^2 (2vq_2 - v^2 - a^2 - 1)^2 - 4(vq_2 + q_2^2)^3 \{ (vq_2 - v^2 - 1)(vq_2 - a^2) - v^2 a^2 \} - \\ & - 4q_2^4 (2vq_2 - v^2 - a^2 - 1)^3 + \\ & + 18q_2(vq_2 + q_2^2)q_2(2vq_2 - v^2 - a^2 - 1) \{ (vq_2 - v^2 - 1)(vq_2 - a^2) - v^2 a^2 \} - \\ & - 27q_2^2 \{ (vq_2 - v^2 - 1)(vq_2 - a^2) - v^2 a^2 \}^2. \end{aligned} \quad (5.1)$$

Proposition 5.2. *i) Suppose $p = 2$ and $q_2 \neq 0$. Then J has always two bound states and two resonances (or virtual states). In the limit $a \rightarrow 0+$, the bound states converge to*

$$\lambda_{1,2}^0 = \pm \sqrt{\left(v + \frac{q_1 - q_2}{2} \right)^2 + 1} + \frac{q_1 + q_2}{2} \quad (5.2)$$

and the resonances converge to

$$\lambda_{3,4}^0 = v + \frac{q_1}{2} \pm \sqrt{\frac{q_1(q_2 q_1 - 4)}{4q_2}}. \quad (5.3)$$

Suppose that $\tilde{v}_1 = v$. Then $\lambda = v$ is always a state.

Moreover, let $D(p_3)$ denote the generalized discriminant given by Formula (5.1). Then, all four states of J are real iff $D(p_3) > 0$. If $D(p_3) < 0$, then there are always two complex conjugated resonances.

ii) Suppose $p = 2$, $\tilde{v}_1 = v$. We have the following asymptotic properties of the states:

- 1) for q_2 small enough, J has precisely two non-real complex conjugated resonances;
- 2) in the limit $q_2 \rightarrow \infty$, the states of J either go to infinity or converge to the real state $\lambda = v$;
- 3) in the limit $v \rightarrow \infty$, the states are of order $|v|$. Moreover, let $\mu_{1,2,3}$ denote the zeros of $\mu^3 - \mu^2 - \mu + q_2 = 0$, which are real if

$$q_2 \in \left[\frac{11 - \sqrt{11^2 + 5 \cdot 27}}{27}, \frac{11 + \sqrt{11^2 + 5 \cdot 27}}{27} \right] \quad (5.4)$$

and contain one complex conjugate pair otherwise. Then $\lambda_{1,2,3}/v \rightarrow \mu_{1,2,3}$ in the limit $v \rightarrow \infty$;

4) for v small enough we do not have non-numerical results;

5) in the limit $a \rightarrow 0+$, the two resonances converge to $\lambda = v$.

Some of this results can be generalized to any p (see Theorem 1.4). The fact that $\lambda = v$ is always a state in the special case $p = 2$, $\tilde{v}_1 = v$, can be generalized to any even p (see Lemma 4.5). We proceed now to the proofs.

Proof: From the properties of function F we know that J has always at least two bound states (or eventually virtual states).

For $p = 2$ we have

$$f_0^+(\lambda) = \frac{\xi_+^2}{a^2} \left((\lambda - v_1)((\lambda - v_2)a - a^2 m_+) - a \right), \quad f_0^-(\lambda) = \overline{f_0^+(\bar{\lambda})}.$$

We get $F = \varphi_2 f_0^+ f_0^- =$

$$= \frac{1}{a^2} [(\lambda - v) \{(\lambda - v_1)(\lambda - v_2) - 1\}^2 - \{(\lambda - v_1)(\lambda - v_2) - 1\}(\lambda - v_1)(\lambda^2 - v^2 + a^2 - 1) + (\lambda - v_1)^2 a^2 (\lambda + v)], \quad (5.5)$$

where we used that $m_+ + m_- = 2\Phi/\varphi_2$ and $m_+ m_- = -\vartheta_3/\varphi_2$, where $\varphi_2 = \lambda - v$, $\Phi = (\lambda^2 - v^2 + a^2 - 1)/2a$, $\vartheta_3 = -\lambda - v$.

Suppose $v_1 = v$ and $\lambda \neq v$. From (5.5) we get $\frac{a^2 F(\lambda)}{\lambda - v} =$

$$= -(\lambda^2 - v^2 - a^2 - 1)(\lambda - v)q_2 + (\lambda - v)^2 q_2^2 + a^2 = \quad (5.6)$$

$$= -q_2 \lambda^3 + \lambda^2 (v q_2 + q_2^2) - \lambda q_2 (2v q_2 - v^2 - a^2 - 1) + (v q_2 - v^2 - 1)(v q_2 - a^2) - v^2 a^2 \quad (5.7)$$

As $F(\lambda) = \frac{\lambda-v}{a^2}p_3(\lambda)$ we have: $\text{sign } F = -\text{sign } q_2$ in the limit $\lambda \rightarrow \pm\infty$. As F is strictly negative under the first band and strictly positive over the second band, we have:
if $q_2 < 0$ then there is one bound state in γ_0^+ ; if $q_2 > 0$ then there is one bound state in γ_2^+ ; state $\lambda = v \in \gamma_1$;

the other 2 states are either real, then they belong to the same gap, or complex conjugate.

The right hand side of (5.7) is the cubic polynomial with real coefficients in λ and can have 3 real zeros or one real zero and two complex conjugated zeros. Denote the respective coefficients in (5.7) by k_0, k_1, k_2, k_3 , then we have

$$\frac{a^2 F(\lambda)}{\lambda - v} = p_3(\lambda) = k_0 \lambda^3 + k_1 \lambda^2 + k_2 \lambda + k_3,$$

$$k_0 = -q_2, \quad k_1 = vq_2 + q_2^2, \quad k_2 = -q_2(2vq_2 - v^2 - a^2 - 1), \quad k_3 = (vq_2 - v^2 - 1)(vq_2 - a^2) - v^2 a^2.$$

Remark 3.104 on page 127 from [Vi], states that if the generalized discriminant of p_3

$$D(p_3) = k_1^2 k_2^2 - 4k_1^3 k_3 - 4k_0 k_2^3 + 18k_0 k_1 k_2 k_3 - 27k_0^2 k_3^2 \quad (5.8)$$

is strictly positive then all the zeros of (5.7) are real and distinct. If $D(p_3) < 0$, then there are two complex conjugated zeros. The discriminant $D(p_3)$ is given in (5.1).

Thus we have proven the first part i) of Proposition 5.2 except asymptotics (5.2) and (5.3 which we postpone to the end of this section.

Suppose $q_2 \rightarrow 0$. Then

$$k_0 = -q_2, \quad k_1 = vq_2 + \mathcal{O}(q_2^2), \quad k_2 = q_2(v^2 + a^2 + 1) + \mathcal{O}(q_2^2), \quad k_3 = a^2 + \mathcal{O}(q_2).$$

Then $D = -27k_0^2 k_3^2 + \mathcal{O}(q_2^3) = -27q_2^2 a^4 + \mathcal{O}(q_2^3)$ which implies that there are two non-real resonances.

Suppose $q_2 \rightarrow \infty$. Then directly from the equation

$$-q_2 \lambda^3 + q_2^2 \lambda^2 - 2vq_2^2 \lambda + v^2 q_2^2 = \mathcal{O}(q_2) \Leftrightarrow \lambda^2 - 2v\lambda + v^2 = (\lambda - v)^2 = \mathcal{O}(\lambda^3 q_2^{-1}), \quad q_2 \rightarrow \infty,$$

we get that the states which remain bounded as $q_2 \rightarrow \infty$ converge to v .

Suppose $v \rightarrow \infty$. Then the equation is $-q_2 \lambda^3 + vq_2 \lambda^2 + q_2 v^2 \lambda - v^3 q_2^2 = \mathcal{O}(v^2)$. Put $\lambda = v\mu$, then $-q_2 v^3 (\mu^3 - \mu^2 - \mu + q_2) = \mathcal{O}(v^2) \Leftrightarrow \mu^3 - \mu^2 - \mu + q_2 = \mathcal{O}((vq_2)^{-1})$, $v \rightarrow \infty$. The equation $\mu^3 - \mu^2 - \mu + q_2 = 0$ has the generalized discriminant $D = 1 + 4q_2 + 4 + 16q_2 - 27q_2^2 = -27q_2^2 + 22q_2 + 5$, whose zeros are

$$x_{\pm} = \frac{11 \pm \sqrt{11^2 + 5 \cdot 27}}{27}.$$

Denote $\mu_{1,2,3}$ the zeros of the equation $\mu^3 - \mu^2 - \mu + q_2 = 0$. We proved that, as $v \rightarrow \infty$, the states $\lambda_{1,2,3} = \mathcal{O}(v)$, moreover $\lambda_{1,2,3}/v$ converge to the zeros of the equation $\mu^3 - \mu^2 - \mu + q_2 = 0$, which are real if $q_2 \in [x_-, x_+]$. If $q_2 < x_-$ or $q_2 > x_+$ then the two zeros are complex conjugated. Thus we have proven the part ii) of Proposition 5.2. In the case $v \rightarrow 0$, the equation does not simplify.

Asymptotics (5.2) and (5.3) as $a \rightarrow 0$. As a special case of the asymptotics in Lemma 3.1, we get, for $\lambda \in \gamma_1^+$,

$$\begin{aligned} f_0^+ &= \frac{1}{a^2} \left(\frac{a}{2\delta} + \mathcal{O}(a^3) \right) ((\lambda - v_1) [(\lambda - v_2)a + \mathcal{O}(a^3)] - a) = \\ &= \frac{1}{a^2} \left(\frac{(\lambda - v_1)(\lambda - v_2) - 1}{2\delta} a^2 + \mathcal{O}(a^4) \right) = \frac{(\lambda - v_1)(\lambda - v_2) - 1}{\lambda^2 - v^2 - 1} + \mathcal{O}(a^2). \end{aligned}$$

Thus the bound states in γ_1^+ which are solutions of $f_0^+(\lambda) = 0$ in the limit $a \rightarrow 0$ are asymptotically solutions of the equation

$$\frac{(\lambda - v_1)(\lambda - v_2) - 1}{\lambda^2 - v^2 - 1} = 0 \Leftrightarrow \lambda^2 - (v_1 + v_2)\lambda + v_1v_2 - 1 = 0$$

if $\lambda^2 \neq v^2 + 1$ (which happens if λ is a virtual state). We get two solutions ($\tilde{v}_1 = v + q_1$, $\tilde{v}_2 = -v + q_2$)

$$z_{1,\pm} = \frac{\tilde{v}_1 + \tilde{v}_2 \pm \sqrt{(\tilde{v}_1 - \tilde{v}_2)^2 + 4}}{2} = \pm \sqrt{\left(v + \frac{q_1 - q_2}{2}\right)^2 + 1} \pm \frac{q_1 + q_2}{2}$$

which are the leading terms in the expansion of the bound states in γ_1^+ as $a \rightarrow 0$ (see Theorem 1.3).

Similarly we get the resonances in γ_1^- and states in $\gamma_{0,2}^\pm$ in the limit $a \rightarrow 0$. The resonances in γ_1^- are formally also zeros of $f_0^-(\lambda)$ in γ_1^+ which, if $v_1 \neq v$, in the leading order a^{-2} are solutions of the equation $(v_2 + v)\lambda^2 - (v_2v + v^2 + v_1(v_2 + v))\lambda + v_1(v_2v + v^2 + 1) - v = 0$ with zeros given in (1.11):

$$\mu_{1,2}^0 = \frac{q_2(2v + q_1) \pm \sqrt{q_2q_1(q_2q_1 - 4)}}{2q_2} = v + \frac{q_1}{2} \pm \sqrt{\frac{q_1(q_2q_1 - 4)}{4q_2}}$$

which can be real antibound states or complex conjugated resonances. If $v_1 = v$ then the leading order as $a \rightarrow 0$ of the antibound state is $\lambda = v$. □

Suppose now that λ_0 is a real double root: $F(\lambda_0) = 0$, $\dot{F}(\lambda_0) = 0$. Suppose $\lambda_0 \neq v$. Using the identity

$$a^2 \dot{F}(\lambda) = a^2 \frac{F(\lambda)}{\lambda - v} + (\lambda - v) \frac{\partial}{\partial \lambda} \left(a^2 \frac{F(\lambda)}{\lambda - v} \right),$$

we have at $\lambda = \lambda_0$:

$$a^2 \dot{F}(\lambda_0) = (\lambda_0 - v) \frac{\partial}{\partial \lambda} \left(a^2 \frac{F(\lambda)}{\lambda - v} \right) \Big|_{\lambda=\lambda_0} = 0.$$

In the special case $p = 2, v_1 = v$, we get using (5.7):

$$\frac{\partial}{\partial \lambda} \left(a^2 \frac{F(\lambda)}{\lambda - v} \right) \Big|_{\lambda=\lambda_0} = -3q_2\lambda_0^2 + 2q_2(v + q_2)\lambda_0 - q_2(2vq_2 - v^2 - a^2 - 1) = 0.$$

It follows that if $F(\lambda_0) = \dot{F}(\lambda_0) = 0$ and $\lambda_0 \neq v$ then λ_0 is a zero of the quadratic equation $3\lambda^2 - 2(v + q_2)\lambda + (2vq_2 - v^2 - a^2 - 1) = 0$:

$$\lambda_0 = \frac{(v + q_2) \pm \sqrt{(v + q_2)^2 - 3(2vq_2 - v^2 - a^2 - 1)}}{3} = \frac{(v + q_2) \pm \sqrt{(2v - q_2)^2 + 3(a^2 + 1)}}{3}.$$

The state has multiplicity 2 and necessarily are the antibound states as all bound states are simple. Thus we get

Proposition 5.3 (Double antibound state). *Suppose $p = 2$, $v_1 = v$. Operator J has precisely one antibound state at λ_0 of multiplicity 2 iff the discriminant given in (5.1) is zero. Moreover, the double antibound state different from $\lambda = v$ is given by either of the two following formulæ:*

$$\frac{(v + q_2) \pm \sqrt{(2v - q_2)^2 + 3(a^2 + 1)}}{3}.$$

The state $\lambda = v$ is always simple if $a \neq 0$.

Acknowledgement. The authors thank the referee for remarks.

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